Accelerated Strategic Computing Initiative

ASCI at Livermore

University of California • Lawrence Livermore National Laboratory

No. 1 - January 2001

Some Highlights of the First Five Years of ASCI Research at LLNL

On September 25, 1995, President Clinton directed DOE to undertake the necessary activities to ensure the safety and performance of the nation's nuclear arsenal in an era of no nuclear testing, no new weapon development, a production complex with reduced capacity and capability, and an aging weapons stockpile. The Stockpile Stewardship Program, of which ASCI represents one key component, is DOE's response to this challenge.

The problems that ASCI will solve for science-based stockpile stewardship span the activities and responsibilities of the three Defense Programs laboratories (Los Alamos, Sandia, and Lawrence Livermore). The ASCI Program is implemented by project leaders at each of the laboratories and managed by the Office of Strategic Computing and Simulation under the Assistant Secretary for Defense Programs.

Six scientists in LLNL's ASCI Program were asked to comment on what they considered significant accomplishments during the first five years of ASCI research at the Lab. The achievements noted below are not intended to provide an inclusive list. Rather, the six contributors briefly describe ASCI accomplishments for which they have firsthand knowledge.

Tom Adams is the Associate B Division Leader for Computational Physics

The first five years of ASCI have seen significant progress from the applications perspective. We have made major advances in ASCI code projects and have shown that we can use the large-scale parallel ASCI platforms effectively. There has been substantial progress in the development of advanced algorithms to improve the fidelity of the simulations. We also produced new tools for managing and visualizing the unprecedented quantity of information generated in the simulations.

The ability to run large-scale codes efficiently on massively parallel machines with large numbers of processors was demonstrated in the development and use of a parallel nuclear weapons explosion code to accomplish the ASCI Primary Burn Code Milepost. This followed a series of more than ten weapons-related physics and engineering simulation runs that used more than 5000 processors on the IBM Blue Pacific computer. Besides these extraordinary runs, designers are beginning to make large parallel runs with two new multiphysics codes in early-production mode to address stockpile stewardship issues. Other large parallel calculations use a new capability to simulate high explosive deflagration, relevant to nuclear

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David Cooper is Associate Director for Computation and Chief Information Officer at LLNL

ASCI Achievements in the First Five Years

The ASCI Program is probably the most successful high-performance computing program in U. S. history. In less than five years, it has revolutionized the high-performance computing/supercomputing industry. The Top 500 list of the world's fastest computers is headed by the ASCI White system, and the next three positions are also held by ASCI systems (Blue Pacific, Blue Mountain, and Red). The genius of the ASCI platform program was to use commodity parts to assemble computers with thousands of processors. This enabled the DOE to leverage the large corporate investments in hardware and software by chip manufacturers and computer companies.

The recent successes in simulating, for the first time, in three dimensions the primary and secondary components of an ignited nuclear weapon attest to the unprecedented progress of the ASCI Program. These accomplishments were based on the successes of other elements of ASCI research, notably scalable algorithms, programming techniques for thousands of processors, and unparalleled visualization capabilities—to name only a few.

No other high performance computing activity can claim such accomplishments in an entire program, let alone in five years.

weapons safety, by coupling implicit hydrodynamics, thermal transport, and dynamic chemical processes.

We have improved the fidelity of the simulations by implementing sophisticated material models and are evaluating them for stockpile stewardship applications. We have also improved the numerical algorithms, including better radiation-hydrodynamic methods. New methods have made possible advanced simulations with accuracy higher than had been achieved previously. We were able to apply a new parallel multiphysics code to simulate a class of shock-induced material mixing experiments, producing results that agreed with experimental data. We implemented accurate, scalable parallel methods for neutron transport.

Managing and interpreting the immense quantity of data produced in large parallel calculations is a challenge. We developed a full-function visualization capability (parallel MeshTV), which is now in common use for processing terascale data sets. The users analyze large parallel stockpile stewardship simulations and produce displays in user offices and in the Data Assessment Theater. To support robust parallel I/O, we developed a parallel I/O library and format, HDF5, in collaboration with the National Center for Supercomputing Operations (NCSA). HDF5 has been accepted as a de facto national standard and is used at universities, laboratories, and companies across the U.S. In collaboration with Limit Point Systems, Los Alamos, and Sandia, we developed an initial implementation of an I/O library (SAF) based on a mathematical data model for general communication of scientific data.

The accomplishments of the first five years form a base for new advanced development of the codes, algorithms, and tools. We look forward to using the codes on future platforms to support the Stockpile Stewardship Program.

—Tom Adams

Steve Ashby is the Director of the Center for Applied Scientific Computing

We created the Center for Applied Scientific Computing (CASC) as a nexus for LLNL's computational mathematics and computer science research activities. CASC research in multilevel methods has significantly reduced the execution time of several essential SSP codes. The ASCI Institute for Terascale Simulation (ITS), formed within CASC in 1999, has enabled LLNL to broaden considerably its scope of academic collaboration. Last summer, the ITS supported approximately 50 students and 20 faculty, all of whom spent 4–12 weeks in residence working with ASCI computational scientists. In addition, the ITS hosts 8–12 sabbatical and postdoctoral visitors and manages a timely and useful seminar series.

An ASCI team earned the *1999 Gordon Bell Award* for "Best Performance" at Supercomputing '99. A proof-of-principle simulation using more than 24 billion zones was clocked at 1.18 teraOPS (trillion floating operations per second) on 5,832 processors of the IBM RS/6000 SST system. An 8-billion zone long-time simulation, emulating a shock tube experiment at California Institute of Technology, executed for 27,000 time-steps and represented over 300 quadrillion arithmetic operations. The calculations took slightly more than a week, and produced over three terabytes of data.

We developed the computer code *Ardra*, which offers robust scalable solution methods for neutron and radiation transport problems in complex 3-D geometries and supports high resolution in space, energy, and direction. Ardra has demonstrated its capability to solve systems with billions of unknowns on terascale computers with thousands of processors. It recently ran the largest-ever neutron transport calculation on the ASCI Blue SST system (24 billion unknowns, 5760 processors, 4 hours).

We are continuing to develop effective, parallel multigrid methods. CASC researchers, working in collaboration with SSP and academic colleagues, have developed highly effective and fully parallel multigrid methods for the solution of the linear systems that arise within several SSP codes. Our geometric multigrid methods, aimed at those codes that employ structured meshes, have already sped up certain SSP calculations by an order of magnitude. The scalability of these solvers has been demonstrated in a variety of numerical experiments, including the solution of a linear system with more than one billion unknowns on nearly 6000 processors of ASCI Red in under one minute. Our recent research, which is internationally recognized, has focused on the development of algebraic multigrid methods for problems arising on unstructured meshes. Preliminary results here are extremely encouraging and already one of these methods is the solver of choice in an ASCI code.

—Steve Ashby

Elaine Chandler, a B Division designer, is the manager of the Dynamics of Metals Program

The Dynamics of Metals Program is a cross-directorate program involving C&MS, Computation, Engineering, and Physics and Advanced Technologies. The program has two goals: For the short-term, we are striving to elevate LLNL's capability to model plasticity and dynamic failure in metals in the physical regimes of interest to a state-of-the art; in the longer term, we have embarked on a campaign to predict from the atomic structure of metals the plasticity and failure that occur in experimentally inaccessible regimes. We have realized notable successes in both efforts since the inception of the program. We inserted and analyzed anisotropic strength modeling in problems of interest to the stockpile surveillance program. We used actual crystal size and orientation distributions for a finite material specimen to produce 3-D anisotropic material response in a continuum level simulation, thus demonstrating the power and the potential provided by the multiscale modeling approach. We experimentally validated the simulation of the transition to plasticity in single crystals, using our simulation dislocation sources recently discovered by LLNL experiments. In addition, we experimentally validated first-principles calculations of elastic constants in tantalum.

This program is dependent on the availability of large-scale computing platforms. In an earlier era, it would have been impossible to do this work. Our research is also dependent on the ability to do experiments that validate the methodology. LLNL, fortunately, has the resources for both capabilities, plus innovative people who can work together to make a complex project like this succeed.

—Elaine Chandler

John Moriarty is Group Leader for Metals and Alloys in H Division, Deputy Assistant Program Leader for the Physical Data Research Program, and a Discipline Leader for the Dynamics of Metals Program

As part of the ASCI-supported Equation-of-State (EOS) and Dynamics-of-Metals Programs, we are developing powerful new quantum-based computational methodologies to treat the thermodynamic and mechanical properties of complex metals, including plutonium. We have validated a first-principles prediction of the low-temperature EOS for the f-electron metal praseodymium through careful high-pressure experiments. This represents a major first step in treating the correlated motion of f electrons in such metals, which is a critical capability needed to model key phases and phase transitions in plutonium. At the same time, advanced atomistic computer simulations of high-temperature thermal properties and melting in tantalum have led to a prototype multiphase EOS for this metal, which also has been validated by high-pressure experiments. Using the same atomistic simulation techniques, we have further succeeded in resolidifying molten tantalum in both a metastable glassy state and an equilibrium crystalline state for different simulated pressure conditions. This is giving us new insight into the kinetics of phase transitions and the nature of resolidified metals. These accomplishments have put us on course for achieving our stated goal of a first-principles multi-phase EOS for plutonium by FY05.

With regard to mechanical properties, we have developed an improved high-pressure strength model for plutonium, which is based on careful first-principles calculations of the shear elastic modulus. Complementary quantum-based atomistic simulations of dislocation behavior in tantalum have directly verified, for the first time, the assumed linear scaling of strength with the shear modulus at high pressure in current models. We are now on the verge of linking single dislocation properties obtained from such atomistic simulations with mesoscale simulations of plastic flow and dynamic fracture at micron-length scales involving thousands (and possibly millions) of dislocations. This is an essential capability needed in our long-range multiscale-modeling strategy of bridging length scales from atomistic to continuum to predict the macroscopic mechanical properties of real metals from first principles.

—John Moriarty

Doug Post is the Associate Division Leader for Computational Physics for A-Division and the Group Leader for ICF Code Development in X-Division

During the past five years, the A-Program ASCI projects have successfully begun developing a number of ASCI applications codes, including several algorithm R&D projects, and have begun modernizing our existing production codes. This is allowing us to provide the tools needed now and in the future for our directed stockpile work and campaign support. Several specific achievements illustrate our progress in improving the physics and computational algorithms and our ability to utilize the massively parallel ASCI platforms.

We ran a high resolution 3-D hydrodynamics calculation on an ASCI code with 10 million zones on 1024 processors. We installed a new generation of algebraic multigrid, linear solvers into an ASCI code that scale well for massively parallel computers (thousands of processors). These solvers were developed by our Center for Applied Scientific Computing (CASC) and are capable of handling unstructured meshes with large numbers of zones (tens of millions) and high condition numbers (~10^6 to 10^8).

In addition, we developed and ran a parallel implicit Monte Carlo (IMC) radiation transport code on 1000 processors. A new hybrid Monte Carlo (MC) method speeds up the IMC calculation by a factor of 20. Our discrete ordinate radiation transport code now runs on 1000 processors or more with good parallel efficiency and scaling and practical run times.

The inertial confinement fusion code HYDRA successfully ran 3-D large-angle capsule implosions and matched OMEGA Laser experiments at the University of Rochester. It also successfully modeled a complex 3-D hydrodynamics

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This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

shocked sphere instability experiment on OMEGA and is beginning to be used to model laser hohlraum behavior. A legacy hydrodynamics code now runs on 100 symmetric multi-processors (SMPs) with 80% efficiency. We implemented a Navier-Stokes algorithm for direct numerical simulation mix studies in our adaptive mesh refinement (AMR) code. A massively parallel 3-D version of the AMR code has been used to analyze Richtmeyer-Meshkov and Rayleigh-Taylor experiments on Nova.

Our meshing group has successfully generated meshes with up to 500 million zones for 4000 processors with both structured and unstructured meshes. Our mix group has completed the first 3-D high-resolution direct numerical simulation (DNS) of a moderate Reynolds number (3000–7000) Rayleigh-Taylor instability problem with a high order accuracy spectral code. We have implemented a high order shock capturing method in the DNS code to extend the applicability of the code into the compressible regime. Our ASCI Verification and Validation (V&V) group has developed several nonlinear radiation-hydrodynamics analytic and semi-analytic test problems, which are being used to test and verify the ASCI codes.

—Doug Post

Steve Louis is Assistant Department Head for Research and Development in the Scientific Computing and Communications Department and leads ASCI's Problem Solving Environment (PSE) efforts at LLNL.

The High Performance Storage System (HPSS) is a large software development project, begun in 1993 as a Cooperative Research and Development Agreement (CRADA) between government and industry. For the past five years, the ASCI Problem Solving Environment's (PSE) Archival Storage Project has focused on the continuing design, development and deployment of HPSS. Since the inception of HPSS, Dick Watson of LLNL has co-chaired the HPSS Executive Committee. Mark Gary, LLNL PSE Archival Storage Lead, represents LLNL on the Technical Committee. LLNL's HPSS software team leads the design and development of several critical HPSS software components and their efforts ensure ASCI user priorities are accurately represented in new HPSS releases. Testbed and production HPSS systems are deployed and supported in the open and secure LLNL computing environments through Livermore's Data Storage Group.

Although ASCI provides major support, over 20 organizations have contributed to the success of HPSS. The HPSS collaboration is based on the premise that no single organization has the experience and resources to meet all the challenges represented by the growing storage system I/O, capacity, and functionality imbalances present in high-performance computing environments such as ASCI. The HPSS I/O architecture is designed to scale as technology advances, using software and hardware striping to support parallel I/O. The system will support application data transfers from megabytes to gigabytes per second. File scalability must meet the needs of billions of data sets, some potentially terabytes in size, for total storage capacities to tens of petabytes. The system is required to scale geographically to support distributed systems with disparate storage hierarchies. Storage systems located at different sites must also integrate into a single logical system accessible by heterogeneous clients. HPSS received the prestigious *R&D 100 Award* in 1997 and official ISO 9001 certification in 2000. To date, it is the only ASCI PSE software effort to achieve SEI Capability Maturity Model (CMM) Level 3 status. CMM is a de facto standard for assessing and improving software and software processes.

—Steve Louis

Next Issue

In the next issue of *ASCI at Livermore*, Terri Quinn will continue the discussion of the first five years of ASCI achievements by focusing on scientific visualization at LLNL.

ASCI at Livermore is published by the Accelerated Strategic Computing Initiative Program, a division of the Defense and Nuclear Technologies Directorate at Lawrence Livermore National Laboratory. Please send corrections and contributions to Tim Peck, (925) 424-6251 and peck7@llnl.gov.